Electronic Supplementary Information (ESI)

Components of the Interaction Energy of Odd-electron Halogen Bond: An *ab Initio* Study

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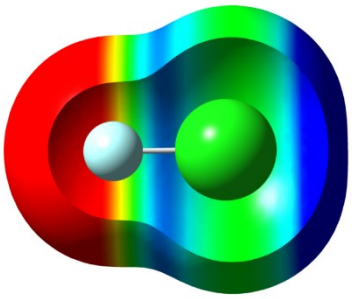
1. Table S1. $V_{S,max}$ on the halogen atoms (in kcal/mol)

Molecule	$V_{S,max}$ on atom	$V_{S,max}$	Molecule	$V_{S,max}$ on atom	$V_{S,max}$
FCl	Cl	47.81	FBr	Br	57.9
ClBr	Cl	20.06	ClBr	Br	37.26
CF_2Cl_2	Cl	22.97	CF_3Cl	Cl	24.48
$CFCl_3$	Cl	21.89	CHF_2Cl	Cl	15.85
$CHFCl_2$	Cl	16.09	CF_3Br	Br	29.88
ClI	I	49.60	ClI	Cl	10.18
CF_3I	I	37.79			

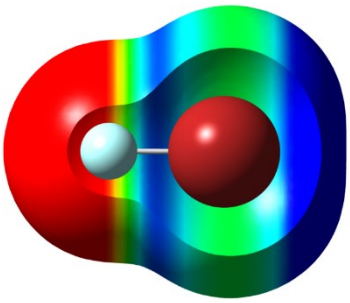
2. Fig.S2. σ-holes on XB donors

Blue colour of the surface represents maximum ESP while red colour corresponds to minimum ESP. Atom Legends: Red: Oxygen, White: Hydrogen, Lime: Chlorine, Cyan: Fluorine, Grey: Carbon, Brown: Bromine, Violet: Iodine

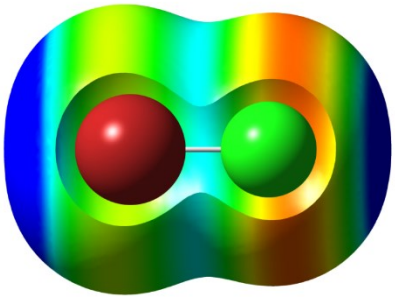
a. FCl



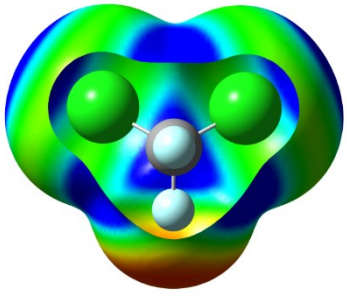
b. FBr



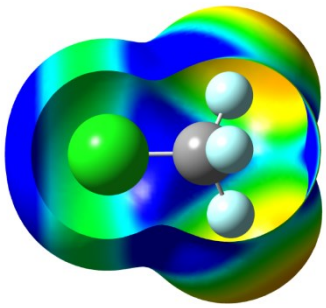
c. ClBr



d. CF_2Cl_2



e. CF_3Cl



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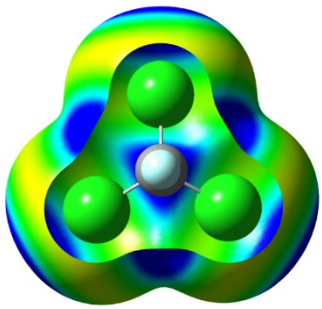
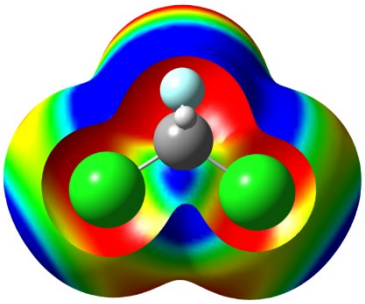
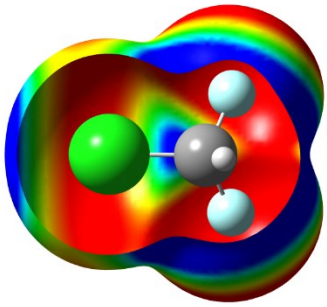


g. $CHFCl_2$



h. CHF_2Cl



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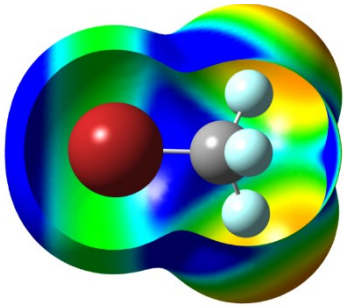

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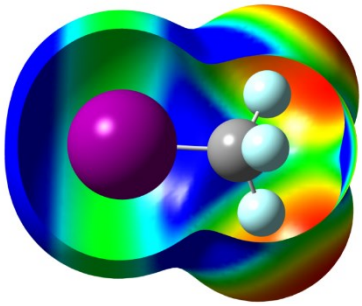

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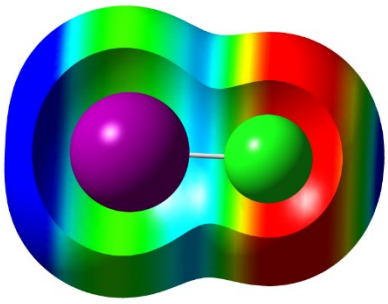


3. Fig S3. Fukui Functions of XB donor molecules

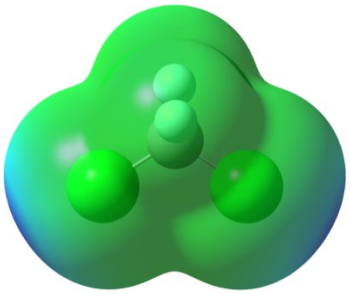
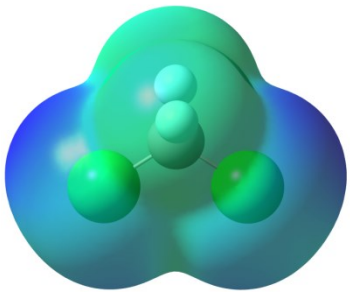
Blue colour of the surface represents maximum Fukui functions. Atom Legends: Red: Oxygen, White: Hydrogen, Lime: Chlorine, Cyan: Fluorine, Grey: Carbon, Brown: Bromine, Violet: Iodine

a.

b.

c.

d.

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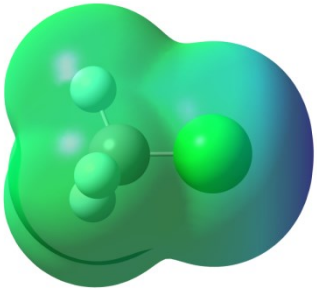
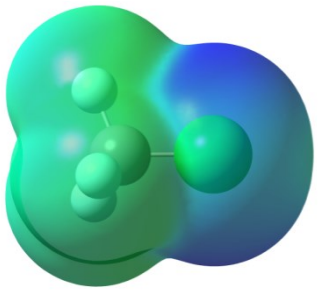

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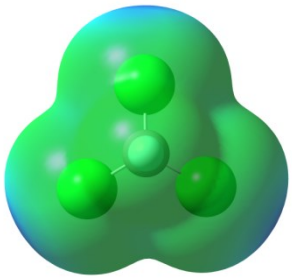
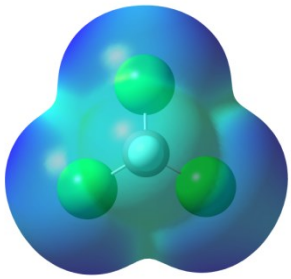

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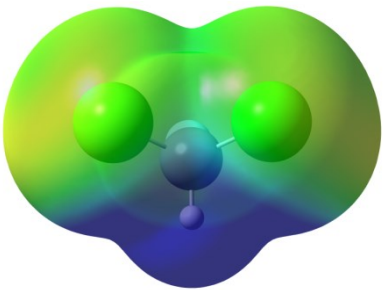
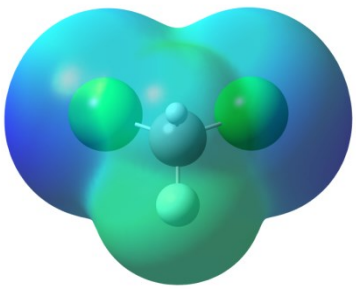

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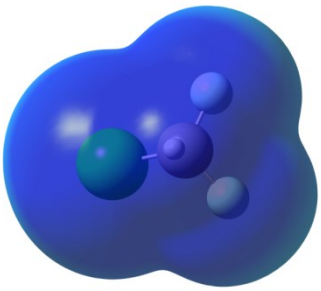
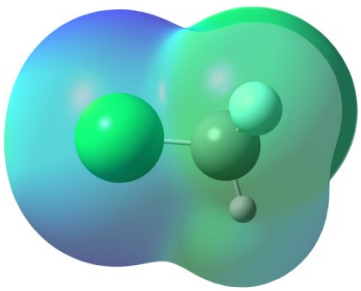

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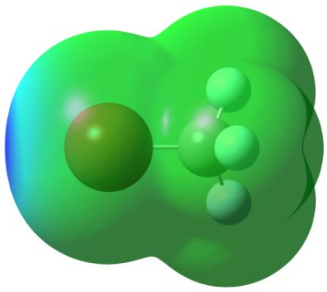

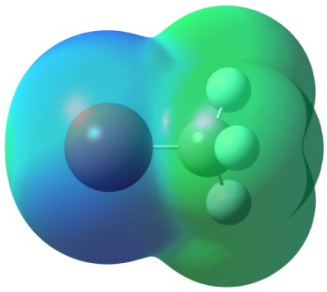

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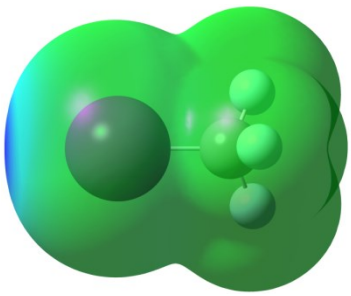

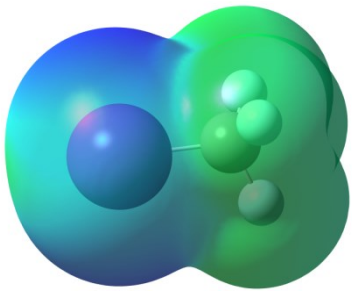

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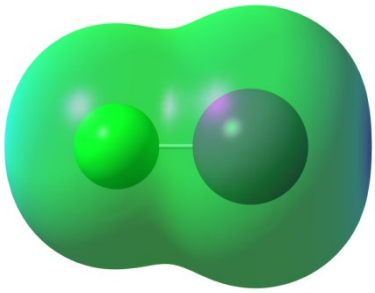
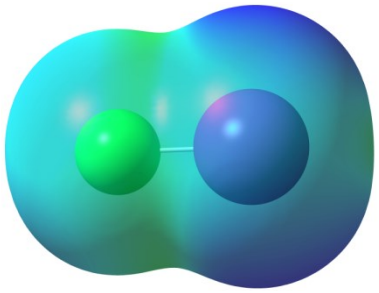


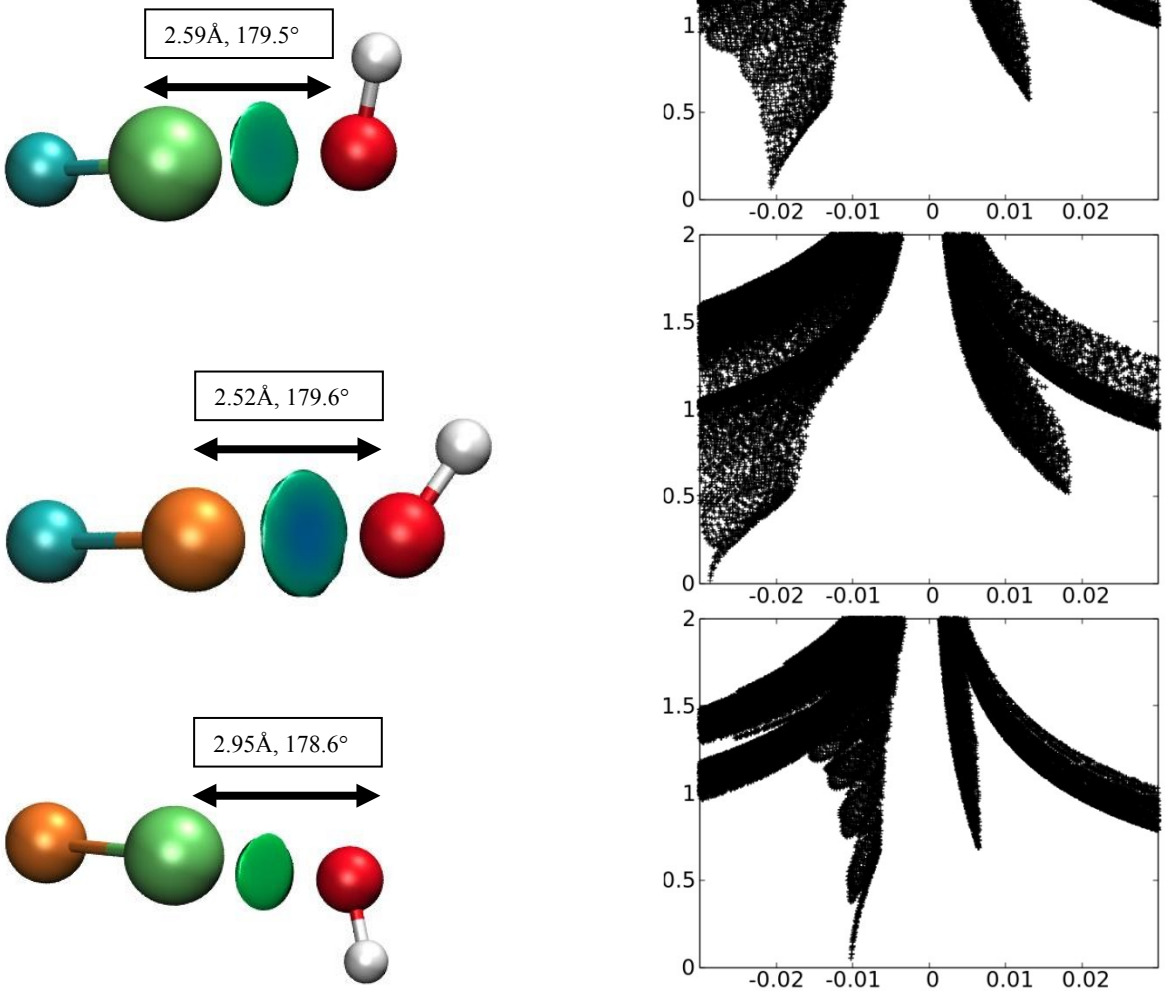


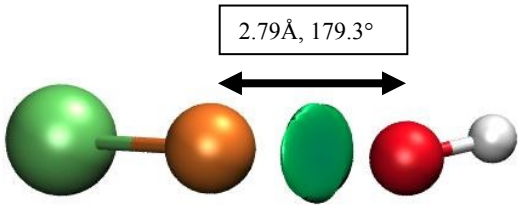
4. Fig S4: NCI iso-surfaces of σ-hole complexes

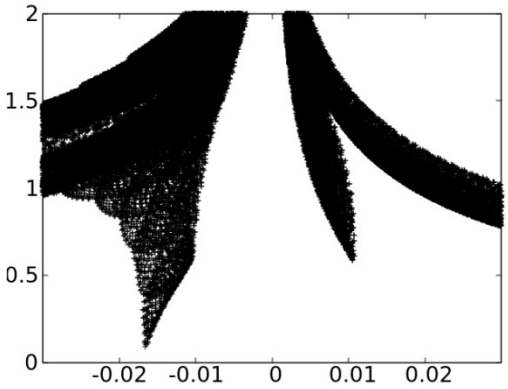
NCI isosurfaces (green and/or bluish green) and NCI index of the radical bound XB complexes. RDG cut-off is 0.5 coloured over -0.2<sign(λ_2)ρ<+0.2 a.u.. Atom Legends: Red: Oxygen, White: Hydrogen, Lime: Chlorine, Cyan: Fluorine, Grey: Carbon, Orange: Bromine, Ochre: Iodine

Axis Codes: X-axis - "sign (λ_2)ρ" and Y-axis- "$s = \frac{1}{\sqrt[3]{2(3\pi^2)}} \frac{|\nabla\rho|}{\rho^{4/3}}$"

a. OH• Complexes




2.79Å, 179.3°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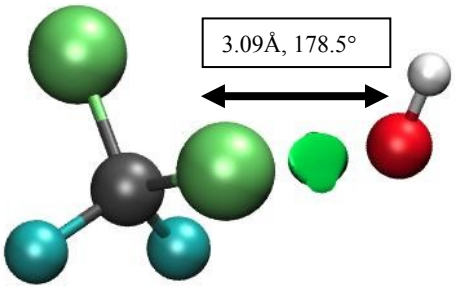
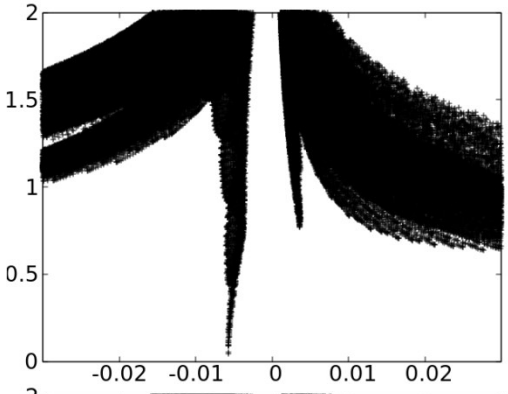

3.09Å, 178.5°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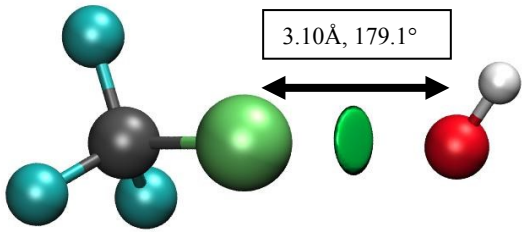
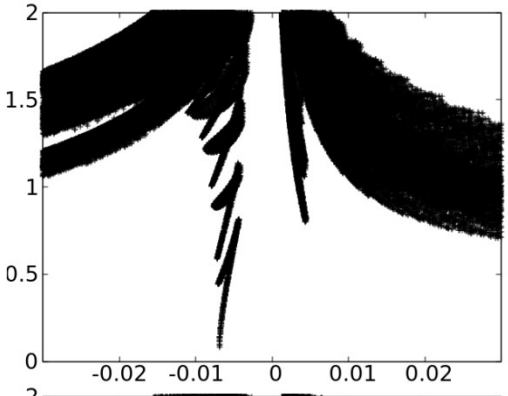

3.10Å, 179.1°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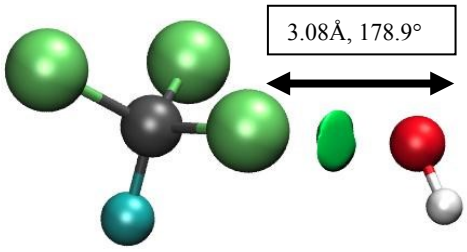
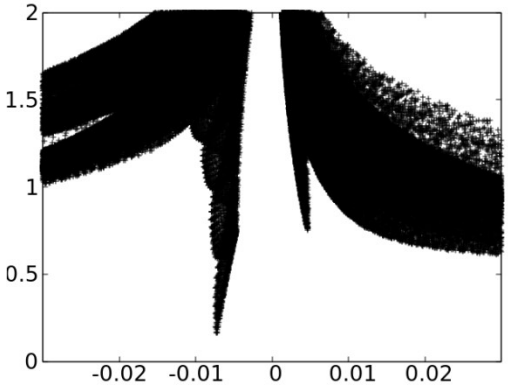

3.08Å, 178.9°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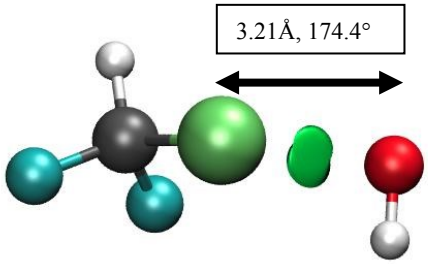
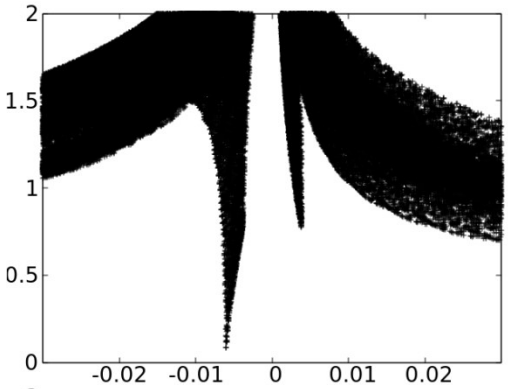

3.21Å, 174.4°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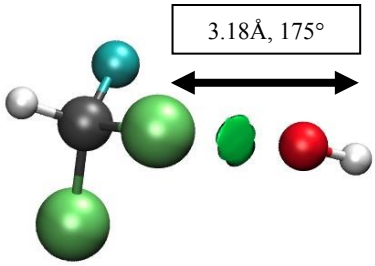
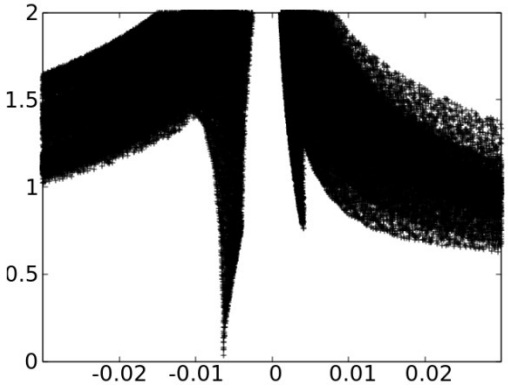

3.18Å, 175°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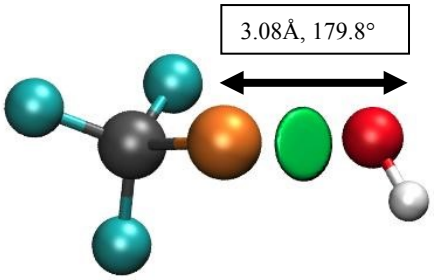
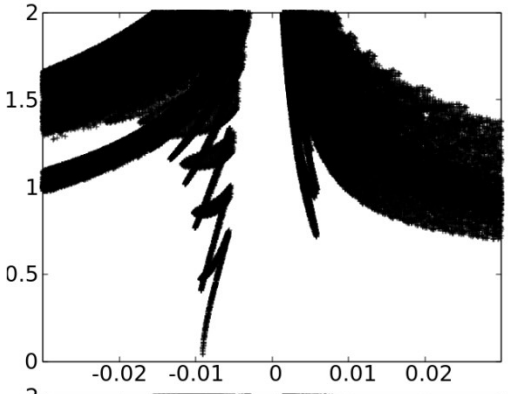

3.08Å, 179.8°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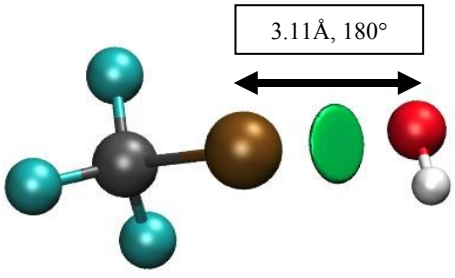
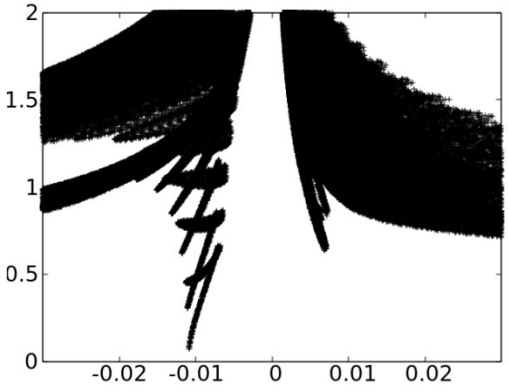

3.11Å, 180°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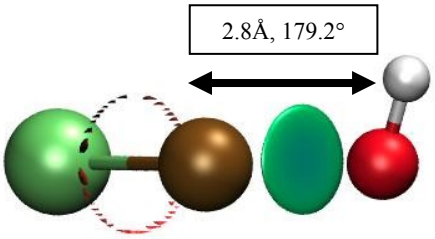
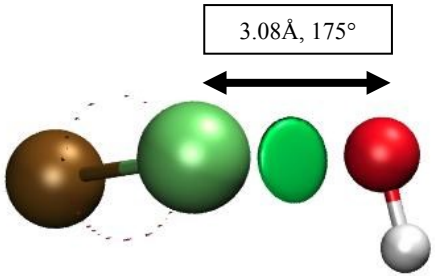
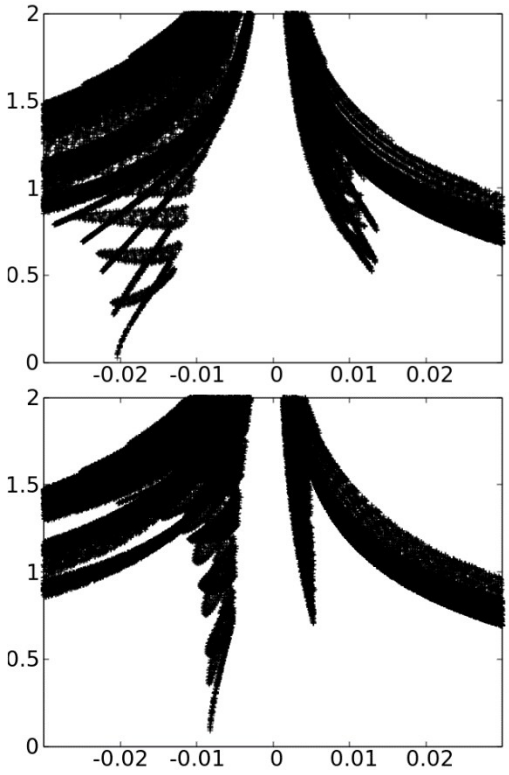

2.8Å, 179.2°


3.08Å, 175°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-0.02
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0
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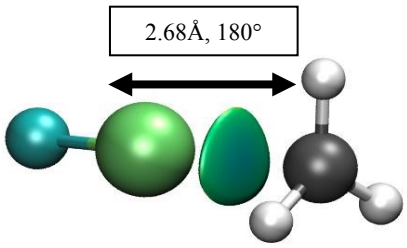
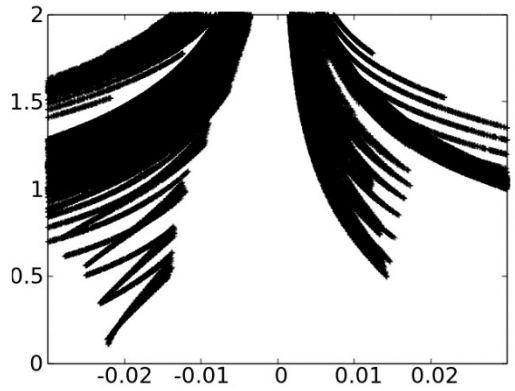
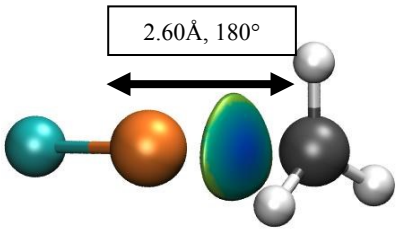
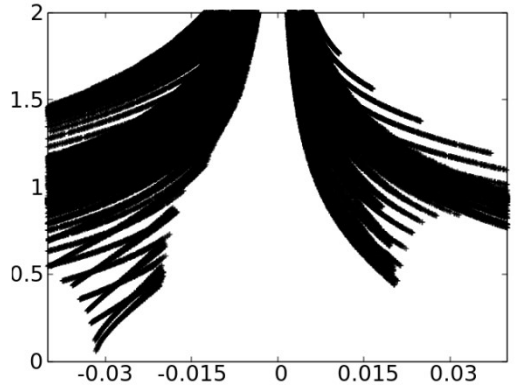
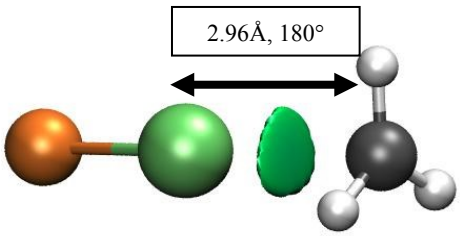
b. CH_3 • Complexes

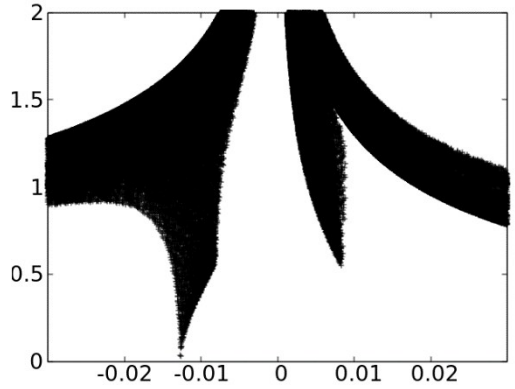


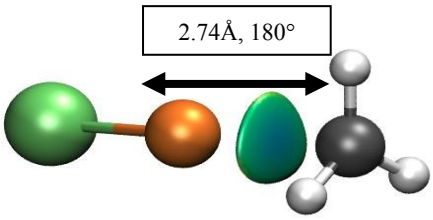


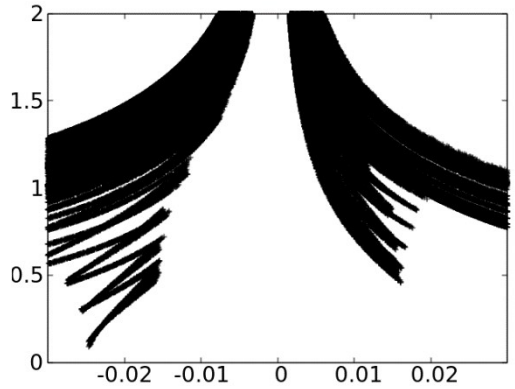


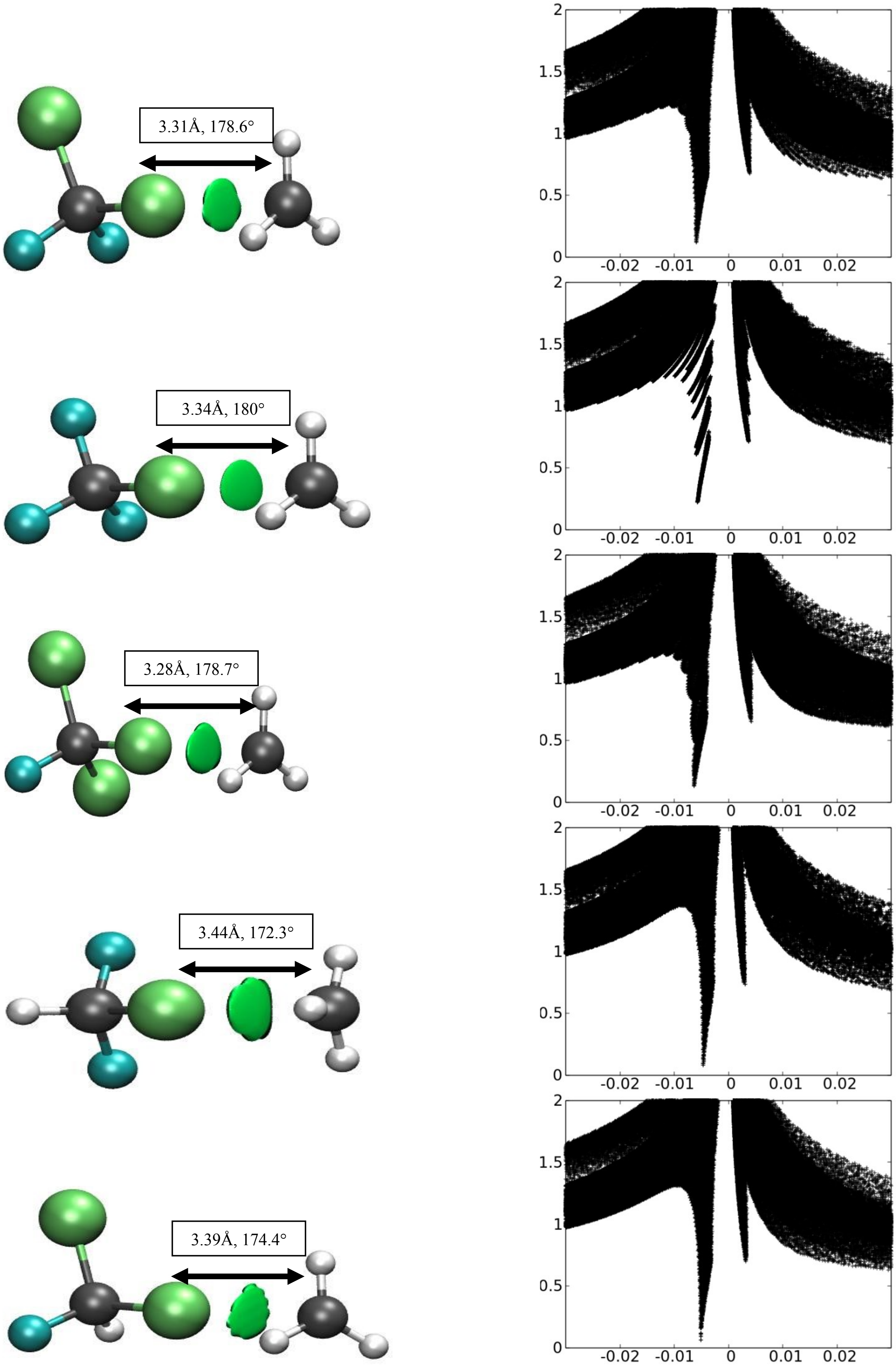


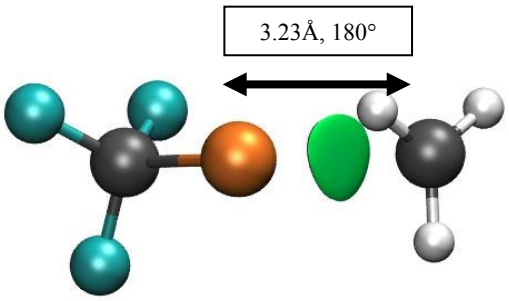









3.31Å, 178.6°
3.34Å, 180°
3.28Å, 178.7°
3.44Å, 172.3°
3.39Å, 174.4°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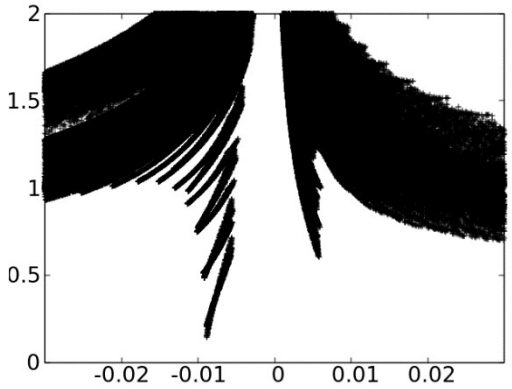
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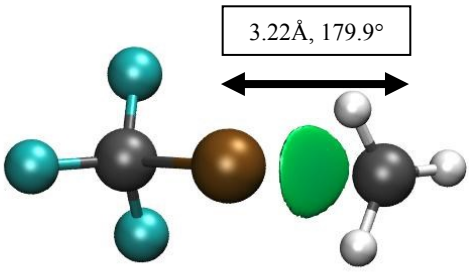
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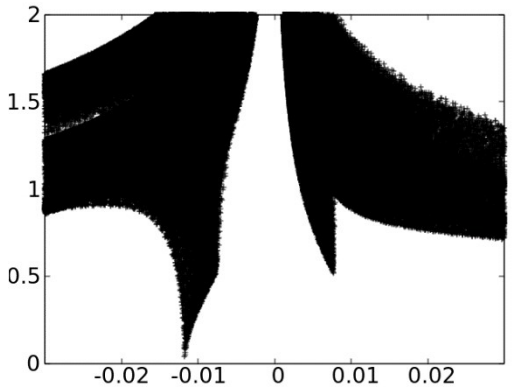
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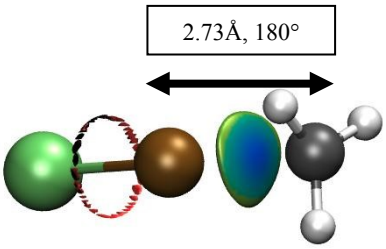
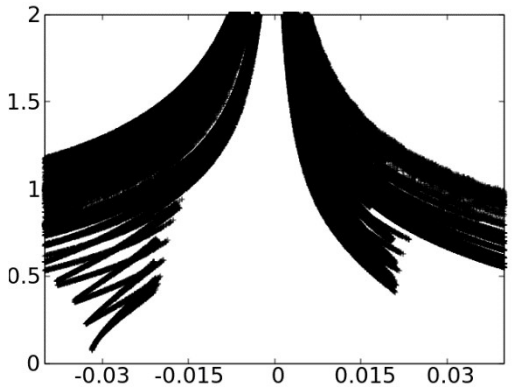

2.73Å, 180°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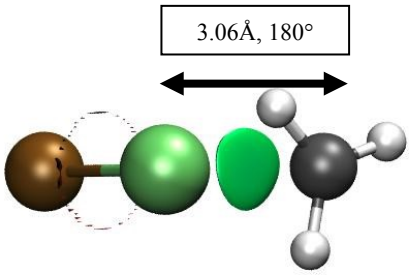
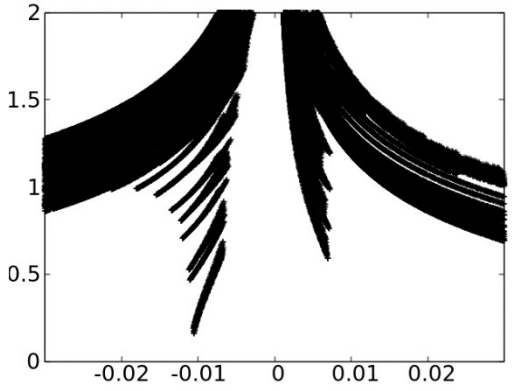

3.06Å, 180°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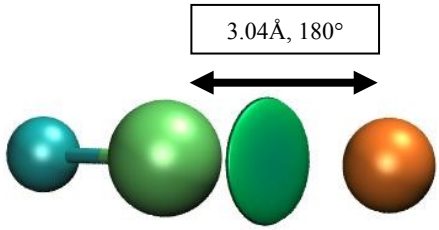
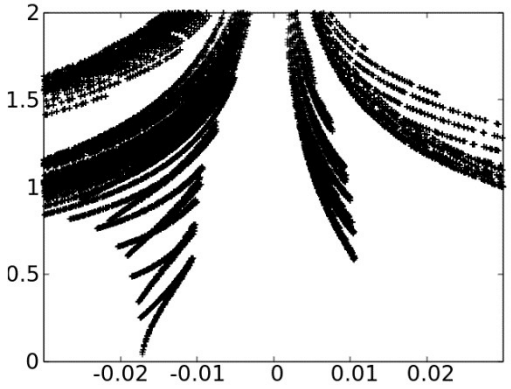
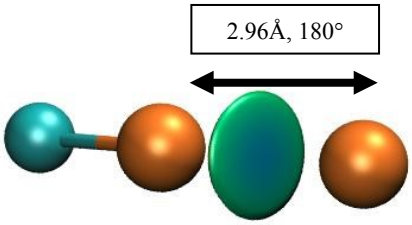
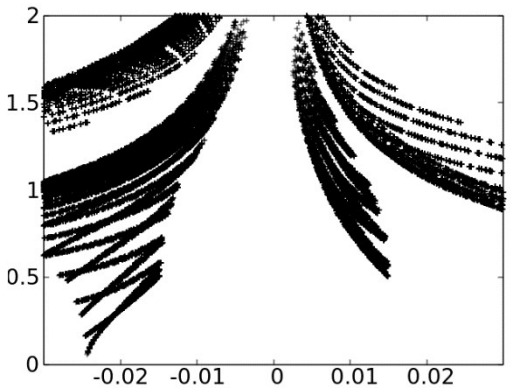
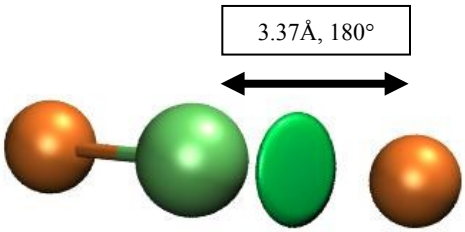
c. Br • Complexes

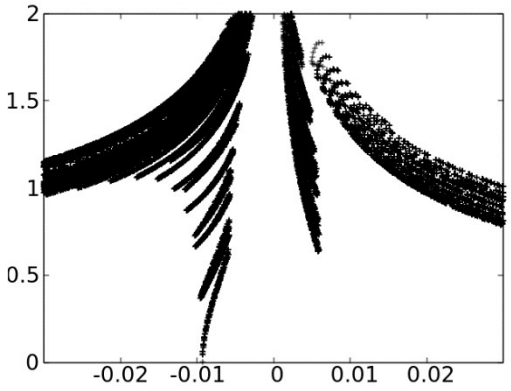


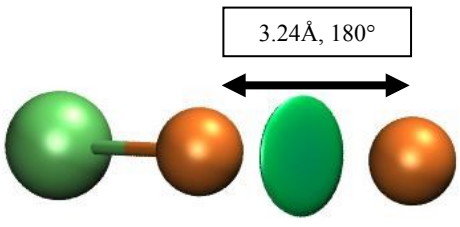


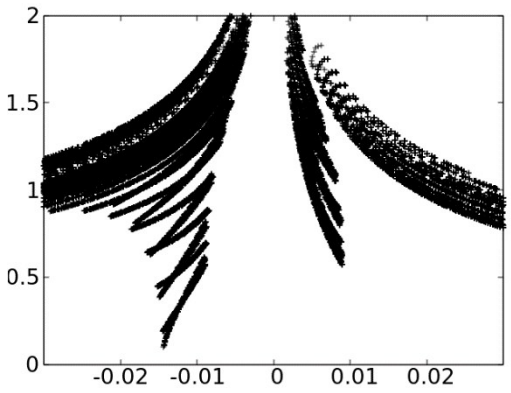


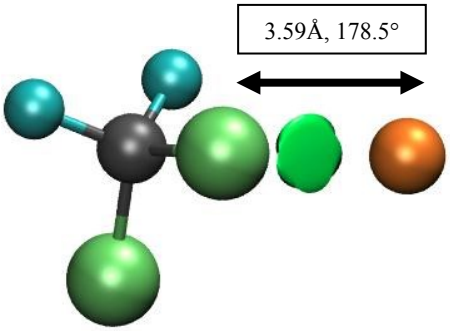


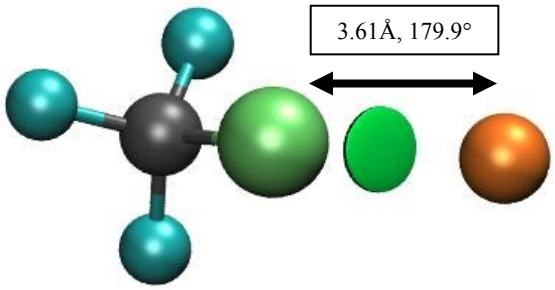


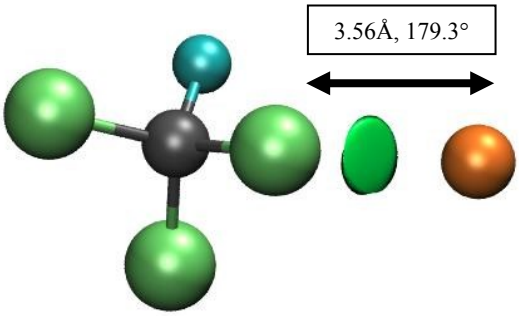


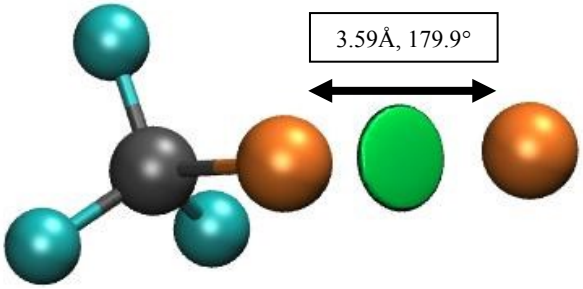





3.59Å, 178.5°


3.61Å, 179.9°


3.56Å, 179.3°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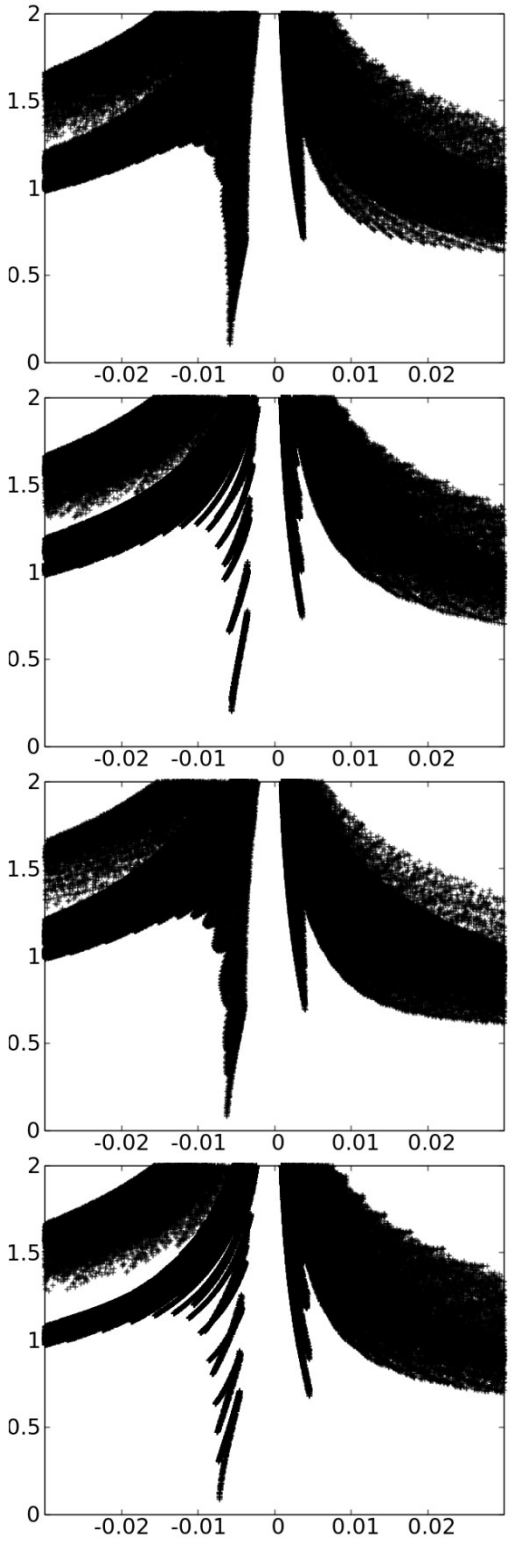
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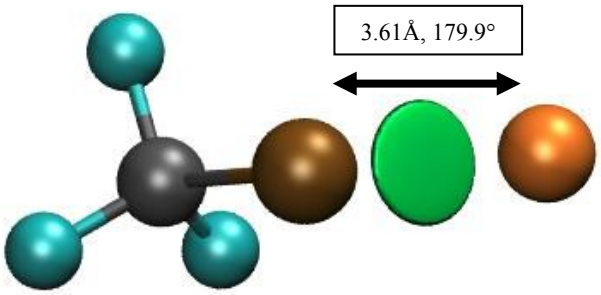
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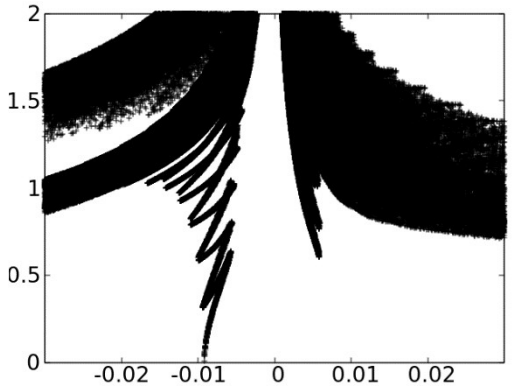
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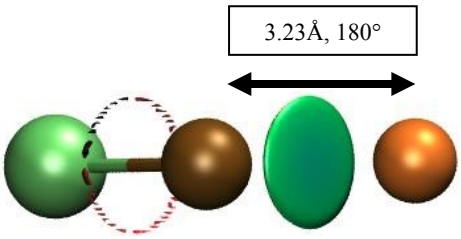
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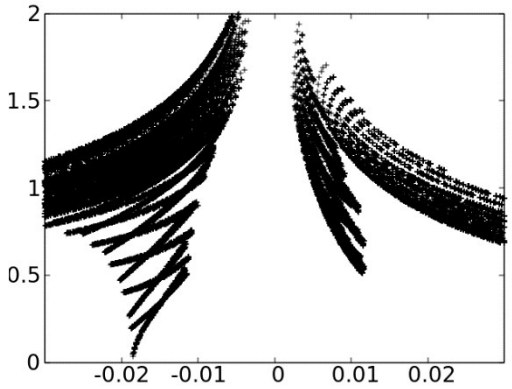
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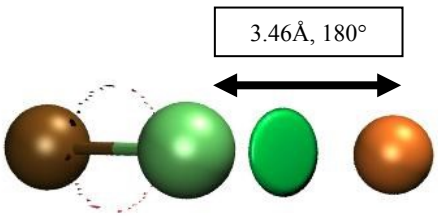
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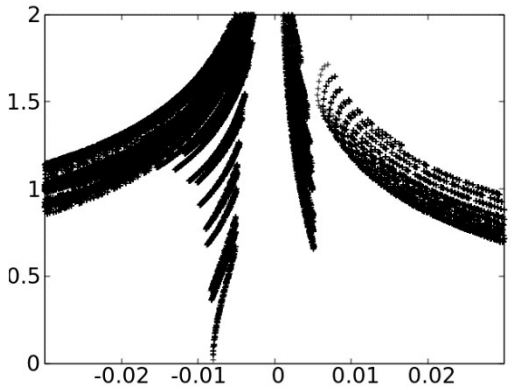
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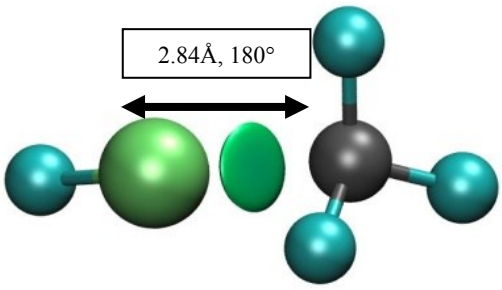
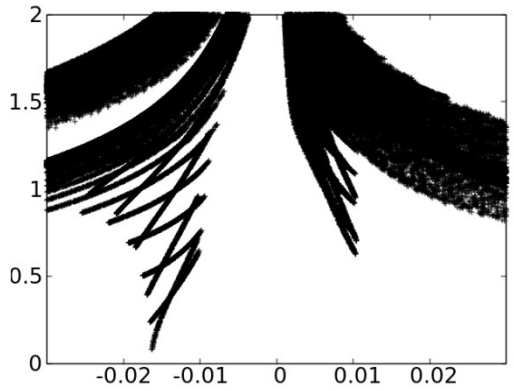
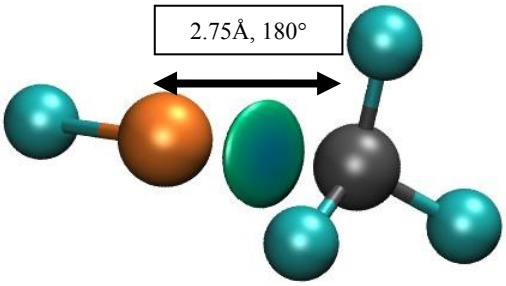
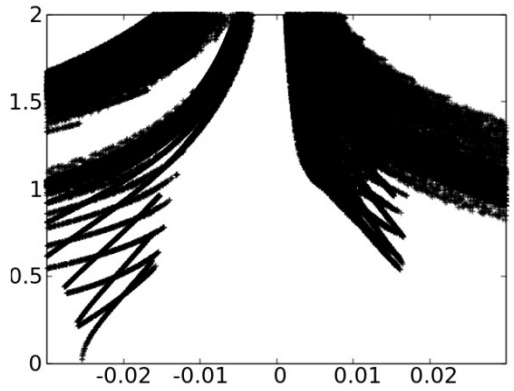
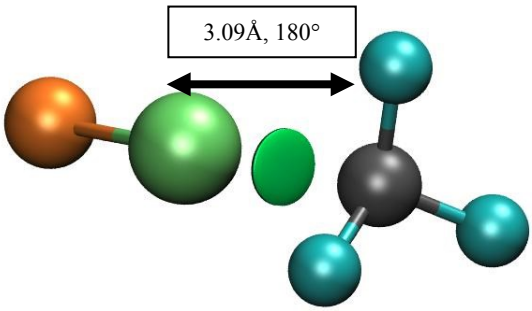
d. $CF_3 \bullet$ Complexes

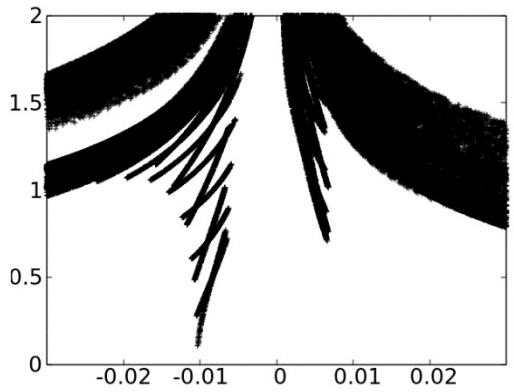


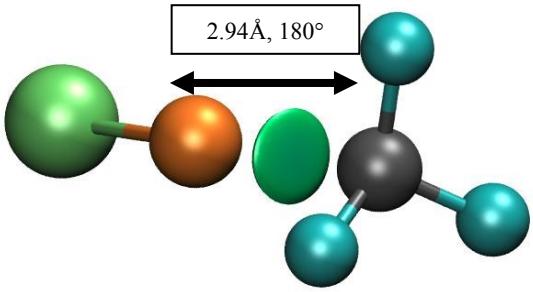


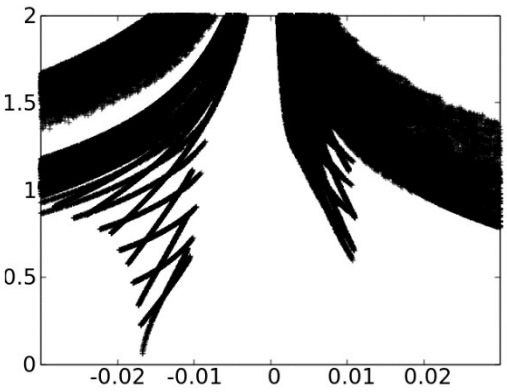


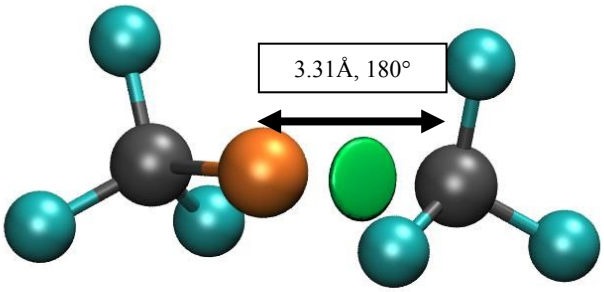


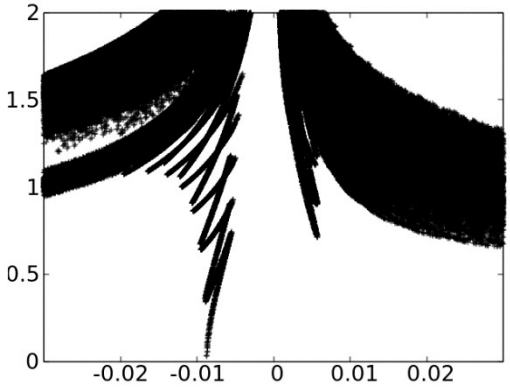









3.31Å, 180°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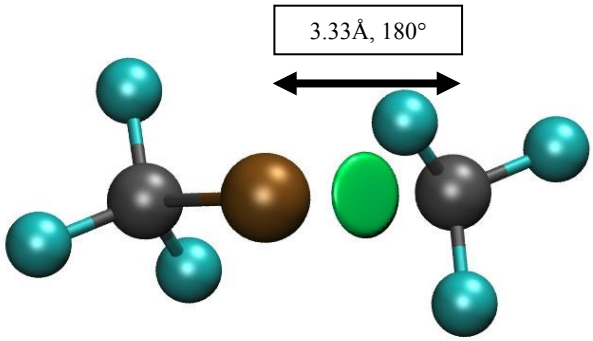
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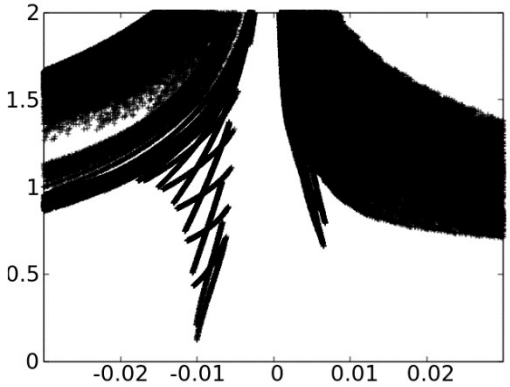
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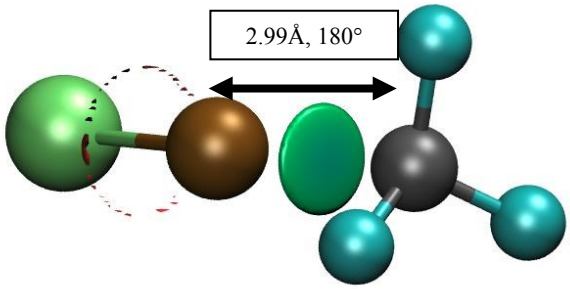
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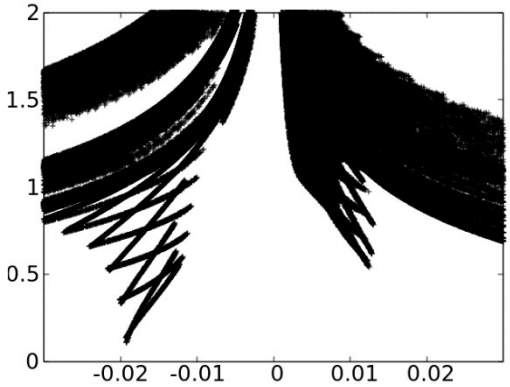
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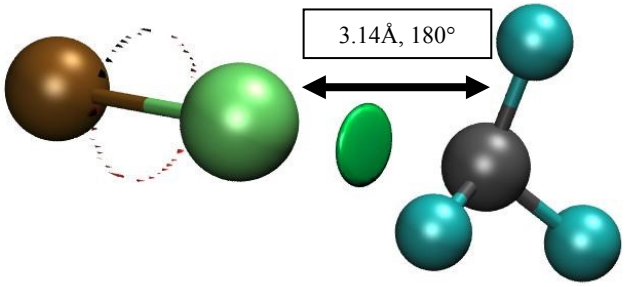
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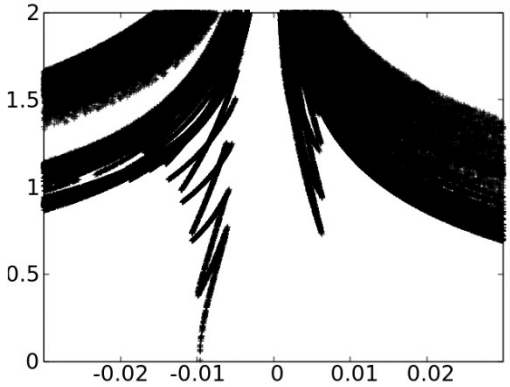
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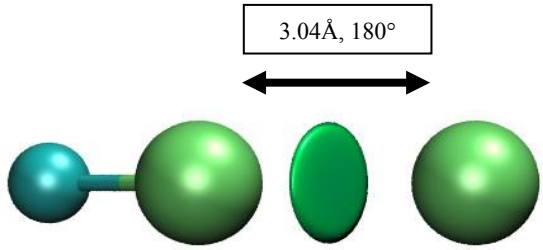
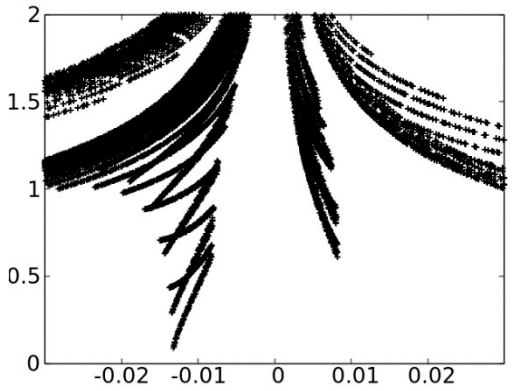
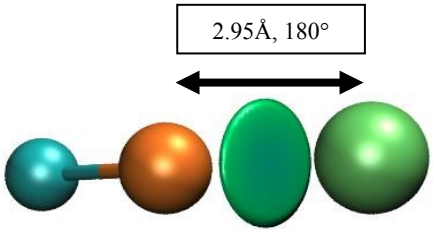
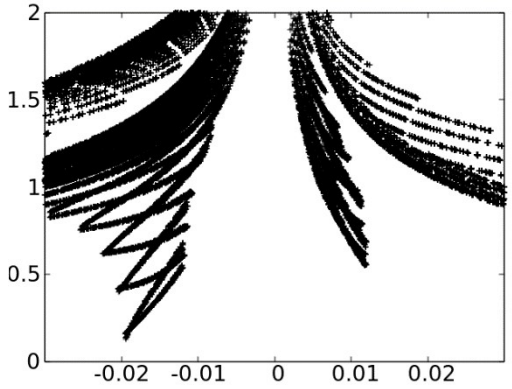
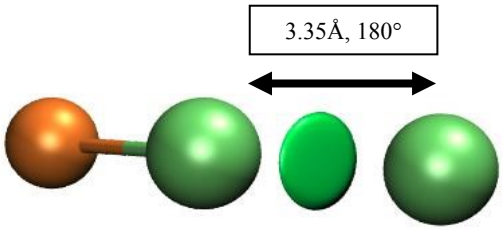
e. Cl • Complexes

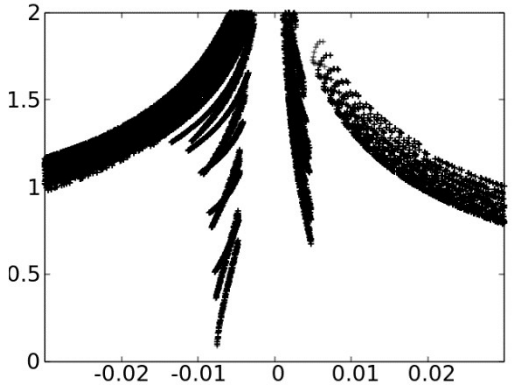


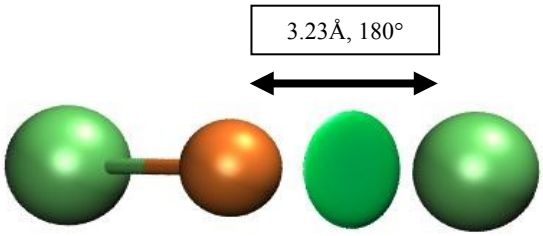


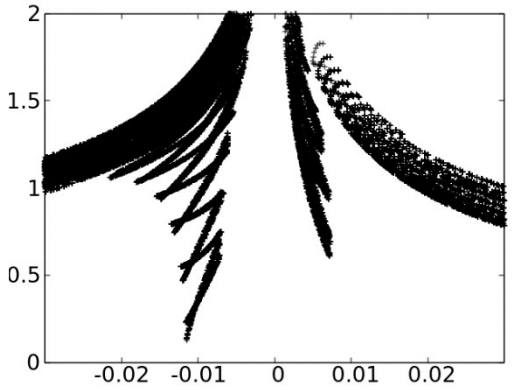


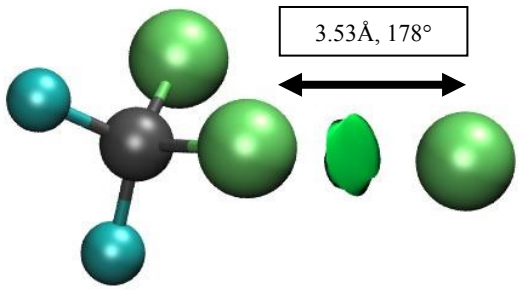


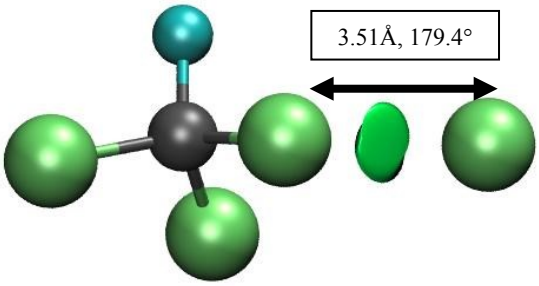


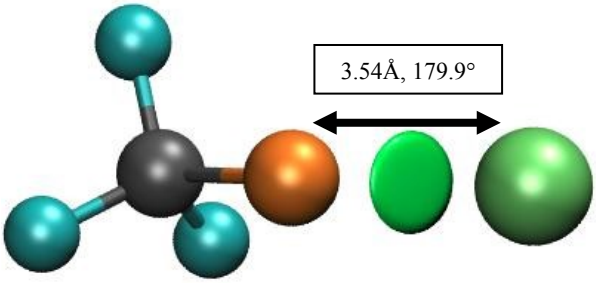


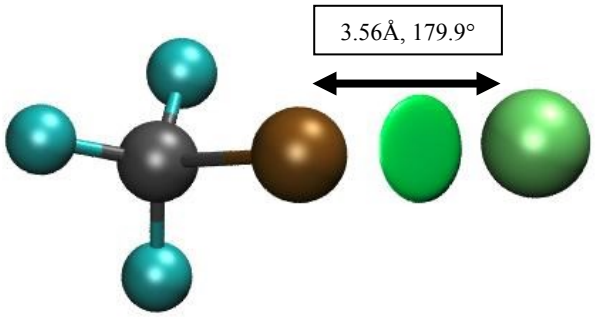


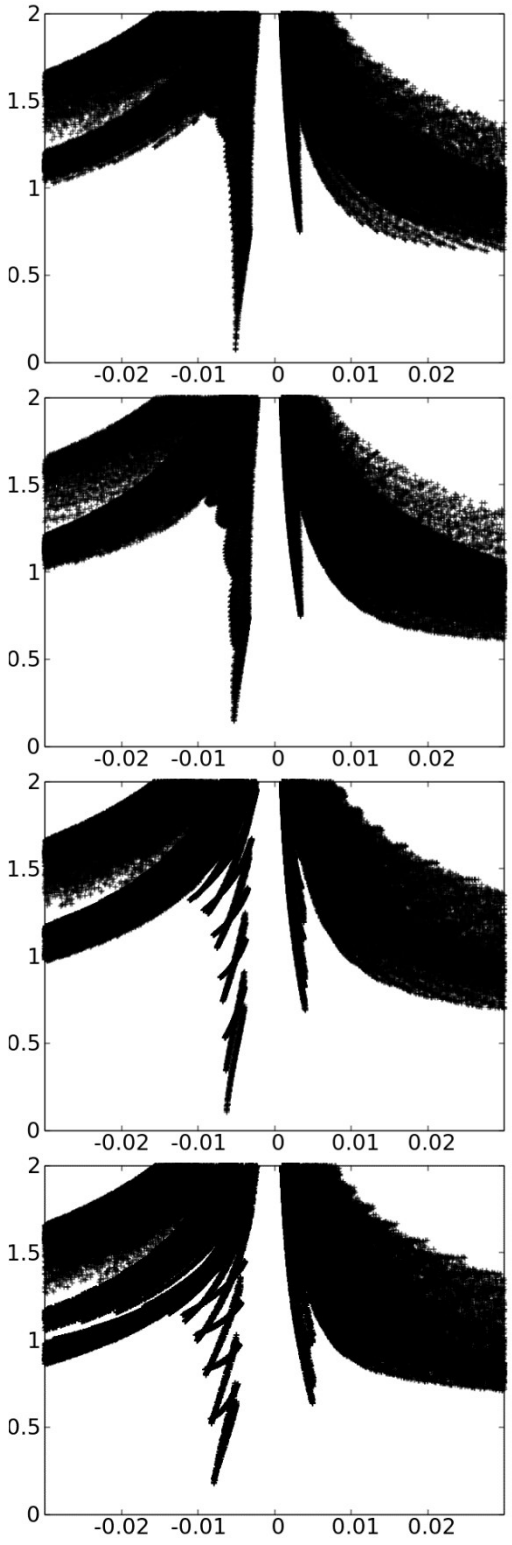


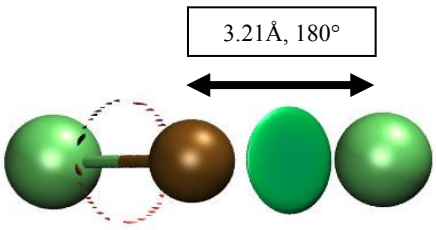

3.53Å, 178°

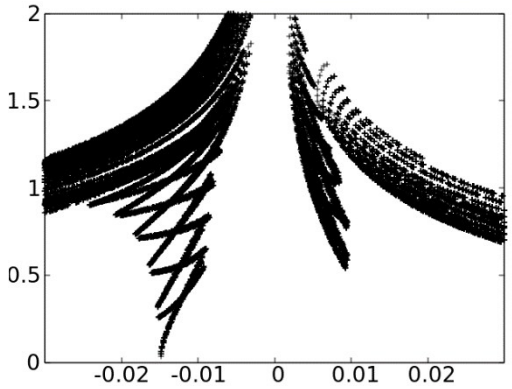

3.51Å, 179.4°

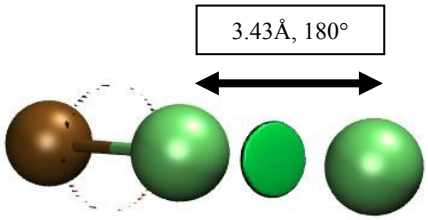

3.54Å, 179.9°

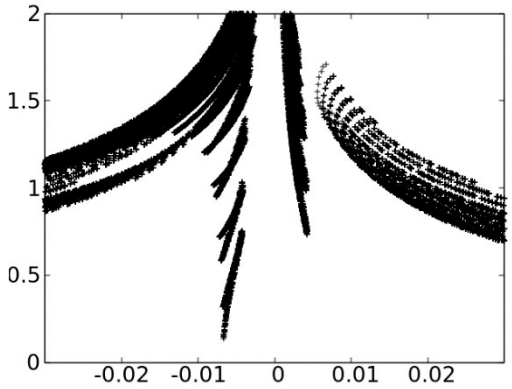

3.56Å, 179.9°


2
1.5
1
0.5
0
-0.02
-0.01
0
0.01
0.02


3.21Å, 180°


2
1.5
1
0.5
0
-0.02
-0.01
0
0.01
0.02


3.43Å, 180°


2
1.5
1
0.5
0
-0.02
-0.01
0
0.01
0.02

5. Table S5: LED analysis of Cl• radical bound complexes

LED analysis of the Cl• radical bound XB interaction. The components of the interaction energies are classified as reference (QRO) and correlation correction by DLPNO-CCSD(T). All units are in kcal/mol. Atomic symbols in Bold denotes the location of sigma-hole unto that atom.

Cl• radical bound complexes										
XB donor	ΔE_{int}	$\Delta E_{geo\text{-}prep}$	Ref. energy decomposition				Corr. energy decomposition			
			ΔE_{int}^{ref}	$\Delta E_{el-prep}^{ref}$	E_{elst}	E_{exch}	$\Delta E_{int}^{C-CCSD(T}$	ΔE_{Disp}^{C-CCSD}	$\Delta E_{no-Disp}^{C-CCSD}$	$\Delta E_{int}^{C-(T)}$
F**Cl**	-1.452	0.020	0.654	33.808	-27.012	-6.142	-2.106	-2.001	0.189	-0.295
F**Br**	-2.199	0.020	0.989	77.879	-63.850	-13.040	-3.188	-2.935	0.188	-0.441
ClBr	-1.682	0.019	0.764	14.056	-10.847	-2.445	-2.446	-3.501	0.214	-0.158
Cl**Br**	-1.187	0.046	0.939	32.870	-26.369	-5.563	-2.215	-2.015	0.155	-0.266
CF_2**Cl_2**	-0.473	0.000	0.379	6.477	-4.946	-1.153	-0.852	-1.022	0.190	-0.020
CF**Cl_3**	-0.514	0.000	0.435	6.997	-5.309	-1.253	-0.949	-1.092	0.179	-0.036
CF_3**Br**	-0.357	0.006	0.449	10.930	-8.640	-1.841	-0.805	-1.205	0.381	0.019
CF_3**I**	-0.715	0.006	0.538	16.317	-12.574	-3.205	-1.253	-1.645	0.400	-0.008
Cl**I**	-2.136	0.046	0.996	52.929	-41.510	-10.423	-3.133	-2.762	0.046	-0.417
ClI	-0.424	0.011	0.831	10.502	-7.762	-1.909	-1.255	-1.272	0.154	-0.137

6. Table S6: LED analysis of CF_3• radical bound complexes

LED analysis of the CF_3 radical bound XB interaction. The components of the interaction energies are classified as reference (QRO) and correlation correction by DLPNO-CCSD(T). All units are in kcal/mol. Atomic symbols in Bold denotes the location of sigma-hole unto that atom.

CF_3• radical bound complexes										
XB donor	ΔE_{int}	$\Delta E_{geo\text{-}prep}$	Ref. energy decomposition				Corr. energy decomposition			
			ΔE_{int}^{ref}	$\Delta E_{el-prep}^{ref}$	E_{elst}	E_{exch}	$\Delta E_{int}^{C-CCSD(T}$	ΔE_{Disp}^{C-CCSD}	$\Delta E_{no-Disp}^{C-CCSD}$	$\Delta E_{int}^{C-(T)}$
F**Cl**	-1.096	-0.058	2.828	61.013	-46.088	-12.097	-3.924	-2.428	-1.015	-0.481
F**Br**	-2.200	-0.175	4.777	155.240	-122.205	-28.258	-6.977	-3.477	-2.708	-0.792
ClBr	-0.595	0.004	1.614	30.888	-23.651	-5.623	-2.209	-1.701	-0.282	-0.227
Cl**Br**	-1.173	-0.015	3.385	77.739	-60.412	-13.941	--4.558	-2.660	-1.422	-0.475
CF_3**Br**	-0.082	0.002	1.616	22.618	-16.808	-4.196	-1.699	-1.361	-0.279	-0.059
CF_3**I**	-0.429	-0.013	2.405	31.441	-21.791	-7.244	-2.835	-1.933	-0.751	-0.151

ClI	-1.917	-0.055	4.433	95.134	-70.358	-20.343	-6.350	-3.221	-2.454	-0.675
ClI	-0.659	0.007	1.281	24.330	-18.075	-4.974	-1.940	-1.668	-0.096	-0.177

7. Table S7: XYZ- coordinates of the Complexes

a. OH• radical Complexes

i) F**Cl**

F	-0.20621	-1.89055	0.00000
Cl	0.00000	-0.25407	0.00000
O	0.30354	2.32383	0.00000
H	-0.57244	2.74358	0.00000

ii) F**Br**

F	-0.27054	-1.88813	0.00000
Br	0.00000	-0.13490	0.00000
O	0.36733	2.36473	0.00000
H	-0.50379	2.79699	0.00000

iii) **Cl**Br

Cl	0.00000	0.78880	0.00000
Br	0.06952	-1.35210	0.00000
O	-0.16772	3.73521	0.00000
H	-1.09129	4.03237	0.00000

iv) Cl**Br**

Cl	0.23772	-1.95367	0.00000
Br	0.00000	0.18165	0.00000
O	-0.34451	2.95708	0.00000
H	-1.28528	3.19786	0.00000

v) CF_2**Cl_2**

C	-0.77954	-0.34800	0.00012
F	-1.14001	-1.05154	-1.07667
Cl	-1.64284	1.18553	0.00092
Cl	0.95599	-0.11459	-0.00343
F	-1.13567	-1.05020	1.07921
O	4.03669	0.21887	0.00514
H	4.54135	1.04664	-0.02203

vi) CF_3**Cl**

C	-1.03988	0.00330	-0.00001
F	-1.49606	1.25214	-0.00377
Cl	0.70663	-0.01184	0.00007
F	-1.51257	-0.61110	1.07951
F	-1.51252	-0.61758	-1.07583
O	3.81048	-0.08592	-0.00004
H	4.43305	0.65771	-0.00002

vii) CF**Cl_3**

C	-0.62314	0.00001	0.26889
F	-0.88979	0.00003	1.58774
Cl	1.11852	0.00001	0.04704
Cl	-1.34041	1.44648	-0.43889
Cl	-1.34039	-1.44650	-0.43884
O	4.19004	-0.00012	-0.28298
H	4.78530	0.00084	0.48279

viii) CHF_2**Cl**

C	1.28629	-0.00010	0.31529
Cl	-0.46911	0.00076	0.27076
F	1.75808	1.08598	-0.32058
F	1.75701	-1.08698	-0.31999
H	1.62727	0.00002	1.34541
O	-3.65967	-0.00052	-0.12307
H	-3.72860	0.00087	-1.09048

ix) CHF**Cl_2**

C	-0.92060	0.45197	0.36985
Cl	-1.83689	-0.96765	-0.13097
F	-1.24409	1.49226	-0.43231
H	-1.18810	0.69068	1.39253
Cl	0.80943	0.16362	0.28328
O	3.92390	-0.34032	-0.14969
H	3.98419	-0.44169	-1.11240

x) CF_3**Br**

C	1.29301	0.00907	0.00016
Br	-0.61437	-0.01809	-0.00038
F	1.77094	-0.64977	1.05168
F	1.77026	-0.56133	-1.10217
F	1.74396	1.25951	0.05135
O	-3.69664	-0.07277	0.00059
H	-4.24837	0.72513	0.00002

xi) CF_3**I**

I	-0.57293	0.01706	-0.00008
C	1.55339	-0.01301	0.00005
F	2.02151	-0.55499	1.12477
F	2.01925	-0.72655	-1.02553
F	2.04720	1.22114	-0.09897
O	-3.69110	0.05917	0.00018
H	-4.21791	-0.75590	0.00005

xii) Cl**I**

I	0.17902	-0.02067	-0.00000
Cl	-2.15613	0.03864	0.00000
O	2.97852	-0.05162	0.00000
H	3.33792	0.85150	0.00000

xiii) **Cl**I

I	0.00000	-1.11582	0.00000

Cl	0.08861	1.20528	0.00000
O	-0.06017	4.28317	0.00000

b. CH_3• radical Complexes

i) F**Cl**

F	-1.91980	0.00000	-0.00000
Cl	-0.27238	-0.00000	0.00000
C	2.40952	0.00000	0.00000
H	2.48373	0.99864	0.39433
H	2.48387	-0.84080	0.66767
H	2.48387	-0.15781	-1.06200

ii) F**Br**

F	-1.92029	-0.00000	0.00000
Br	-0.14710	0.00000	0.00000
C	2.45837	-0.00000	0.00000
H	2.56032	-1.06404	0.13165
H	2.56032	0.41801	-0.98730
H	2.56032	0.64603	0.85566

iii) **Cl**Br

Cl	-0.06187	0.21655	0.75998
Br	0.10569	-0.36993	-1.29825
C	-0.29334	1.02667	3.60299
H	-0.48891	0.01434	3.90891
H	0.71365	1.40424	3.61075
H	-1.11225	1.68765	3.38132

iv) Cl**Br**

Cl	1.96491	-0.00000	0.00000
Br	-0.19294	0.00000	0.00000
C	-2.93412	-0.00000	-0.00000
H	-3.01524	-1.00402	-0.37953
H	-3.01526	0.17332	1.05927
H	-3.01526	0.83069	-0.67973

v) CF_2**Cl_2**

C	-0.80154	-0.34888	0.00000
F	-1.14778	-1.05635	-1.07781
Cl	-1.67886	1.17401	0.00000
Cl	0.93540	-0.09486	-0.00003
F	-1.14774	-1.05632	1.07785
C	4.23033	0.30646	0.00002
H	4.29853	-0.23227	-0.92808
H	4.29715	-0.22183	0.93420
H	4.13007	1.37705	-0.00606

vi) CF_3**Cl**

C	-1.07010	0.00000	0.00000
F	-1.53411	-0.35867	1.19156
Cl	0.68023	0.00000	0.00000
F	-1.53411	-0.85259	-0.90640
F	-1.53411	1.21126	-0.28516
C	4.02680	0.00000	0.00000
H	4.03898	-0.30991	1.02958
H	4.03898	-0.73669	-0.78319
H	-1.02502	4.38328	0.00000
H	4.03898	1.04660	-0.24640

vii) CF**Cl_3**

C	-0.64817	0.00000	0.26917
F	-0.93611	0.00000	1.58215
Cl	1.10168	0.00003	0.07957
Cl	-1.34839	1.44657	-0.45246
Cl	-1.34835	-1.44660	-0.45245
C	4.37731	-0.00001	-0.20234
H	4.34387	-0.90574	-0.78096
H	4.47163	-0.04902	0.86769
H	4.35076	0.95473	-0.69635

viii) CHF_2**Cl**

C	1.32644	0.00002	0.31559
Cl	-0.43210	-0.00012	0.28158
F	1.79134	1.08636	-0.32213
F	1.79151	-1.08623	-0.32216
H	1.67092	0.00003	1.34455
C	-3.83448	0.00007	-0.24556
H	-3.50721	0.93176	-0.67107
H	-4.50874	-0.00141	0.59183
H	-3.50661	-0.93012	-0.67388

ix) CHF**Cl_2**

C	-0.95466	0.44618	0.37477
Cl	-1.85578	-0.97957	-0.13064
F	-1.29452	1.48954	-0.41461
H	-1.21324	0.67273	1.40251
Cl	0.78075	0.17854	0.27091
C	4.09429	-0.34813	-0.25461
H	4.68518	-0.21716	0.63397
H	3.91453	0.48606	-0.90887
H	3.70201	-1.31835	-0.50164

x) CF_3**Br**

C	-1.30800	0.00000	0.00000
Br	0.60400	0.00000	0.00000
F	-1.77400	-1.24400	-0.03700
F	-1.77400	0.59000	1.09600
F	-1.77400	0.65400	-1.05900
C	3.83700	0.00000	0.00000
H	3.85900	0.56600	-0.91400
H	3.85900	-1.07500	-0.03300
H	3.85900	0.50900	0.94700

xi) CF_3**I**

I	-0.37563	-0.21081	-0.37062
C	1.03345	0.57998	1.01967
F	2.27948	0.40843	0.58006
F	0.83540	1.88462	1.20401
F	0.92409	-0.02636	2.20106
C	-2.50612	-1.40643	-2.47271
H	-3.34084	-1.12339	-1.85572
H	-2.09444	-2.39735	-2.39444

H	-2.17111	-0.74793	-3.25482

xii) Cl**I**

I	-0.19124	0.00000	0.00000
Cl	2.16322	0.00000	-0.00000
C	-2.92184	0.00000	-0.00000
H	-3.03597	0.54329	0.92341
H	-3.03597	0.52806	-0.93221
H	-3.03597	-1.07134	0.00879

xiii) **Cl**I

I	-1.11588	0.00000	0.00000
Cl	1.21084	-0.00000	0.00000
C	4.27889	0.00000	0.00000
H	4.29463	0.77204	0.74828
H	4.29464	-1.03404	0.29447
H	4.29465	0.26201	-1.04275

c. Br• radical Complexes

i) F**Cl**

F	0.00000	0.00000	-3.15482
Cl	0.00000	0.00000	-1.50512
Br	0.00000	0.00000	1.54230

ii) F**Br**

F	0.00000	0.00000	-2.88747
Br	0.00000	0.00000	-1.11154
Br	0.00000	0.00000	1.85404

iii) **Cl**Br

Cl	0.00000	0.00000	-0.49663
Br	0.00000	0.00000	-2.63929
Br	0.00000	0.00000	2.88051

iv) Cl**Br**

Cl	0.00000	0.00000	-3.03515
Br	0.00000	0.00000	-0.88620
Br	0.00000	0.00000	2.36042

v) CF_2**Cl_2**

C	-2.13382	-0.04932	0.00000
F	-2.63384	0.55883	1.07777
Cl	-2.63384	-1.73382	0.00000
Cl	-0.38521	0.10580	0.00000
F	-2.63384	0.55883	-1.07777
Br	3.18674	0.51181	0.00000

vi) CF_3**Cl**

C	-2.41340	-0.00014	-0.00005
F	-2.87566	-1.20938	-0.29526
Cl	-0.66292	0.00107	0.00048
F	-2.87705	0.85947	-0.89958
F	-2.87748	0.34843	1.19416
Br	2.95491	-0.00011	-0.00005

vii) CF**Cl_3**

C	1.88246	0.00001	0.26952
F	2.22078	0.00001	1.57020
Cl	0.12668	0.00002	0.14805
Cl	2.55336	-1.44654	-0.47882
Cl	2.55342	1.44651	-0.47883
Br	-3.43574	0.00000	-0.05674

viii) CF_3**Br**

C	-2.41340	-0.00014	-0.00005
F	-2.87566	-1.20938	-0.29526
Br	-0.66292	0.00107	0.00048
F	-2.87705	0.85947	-0.89958
F	-2.87748	0.34843	1.19416
Br	2.95491	-0.00011	-0.00005

ix) CF_3**I**

I	0.35845	0.00021	-0.00001
C	2.48863	-0.00020	0.00003
F	2.96040	-0.74487	-0.99817
F	2.96021	1.23669	-0.14577
F	2.96058	-0.49236	1.14393
Br	-3.25314	-0.00014	0.00002

x) Cl**I**

I	0.00000	0.00000	0.69833
Cl	0.00000	0.00000	3.03522
Br	0.00000	0.00000	-2.53172

xi) **Cl**I

I	0.00000	0.00000	2.30654
Cl	0.00000	0.00000	-0.01714
Br	0.00000	0.00000	-3.48444

d. CF_3• radical Complexes

i) F**Cl**

F	0.00000	0.00000	3.15496
Cl	0.00000	0.00000	1.51508

C	0.00000	0.00000	-1.32512
F	0.00000	1.25557	-1.71112
F	1.08735	-0.62778	-1.71112
F	-1.08735	-0.62778	-1.71112

ii) F**Br**

F	0.00000	0.00000	2.85500
Br	0.00000	0.00000	1.09500
C	0.00000	0.00000	-1.63100
F	0.00000	1.25500	-2.00900
F	1.08700	-0.62800	-2.00900
F	-1.08700	-0.62800	-2.00900

iii) **Cl**Br

Cl	0.00000	0.00000	0.44500
Br	0.00000	0.00000	2.58500
C	0.00000	0.00000	-2.64900
F	0.00000	1.25600	-3.04300
F	1.08700	-0.62800	-3.04300
F	-1.08700	-0.62800	-3.04300

iv) Cl**Br**

Cl	0.00000	0.00000	2.98118
Br	0.00000	0.00000	0.83768
C	0.00000	0.00000	-2.10712
F	0.00000	1.25559	-2.49466
F	1.08737	-0.62779	-2.49466
F	-1.08737	-0.62779	-2.49466

v) CF_3**Br** ****Imported from Ref** [27] ******

Br	0.00000	0.00000	0.43763
C	0.00000	0.00000	2.35208
F	0.00000	1.24447	2.81279
F	-1.07774	-0.62223	2.81279
F	1.07774	-0.62223	2.81279
C	0.00000	0.00000	-2.87464
F	1.08767	-0.62797	-3.26888
F	0.00000	1.25594	-3.26888
F	-1.08767	-0.62797	-3.26888

vi) CF_3**I**

I	0.00000	0.00000	0.31505
C	0.00000	0.00000	2.44706
F	0.00000	1.24534	2.91453
F	-1.07850	-0.62267	2.91453
F	1.07850	-0.62267	2.91453
C	0.00000	0.00000	-3.01511
F	0.00527	-1.25592	-3.40674
F	-1.09029	0.62339	-3.40674
F	1.08502	0.63252	-3.40674

vii) Cl**I**

I	0.00000	0.00000	0.67531
Cl	0.00000	0.00000	3.00316
C	0.00000	0.00000	-2.31824
F	0.00000	1.25536	-2.70133
F	1.08717	-0.62768	-2.70133
F	-1.08717	-0.62768	-2.70133

viii) **Cl**I

I	2.23896	0.00008	0.00002
Cl	-0.08398	-0.00004	0.00003
C	-3.22830	-0.00008	-0.00004
F	-3.62466	-0.74627	-1.00997
F	-3.62471	-0.50165	1.15112
F	-3.62482	1.24759	-0.14127

e. Cl• radical Complexes

i) F**Cl**

F	0.00000	0.00000	-2.50511
Cl	0.00000	0.00000	-0.86045
Cl	0.00000	0.00000	2.18668

ii) F**Br**

F	0.00000	0.00000	2.33179
Br	0.00000	0.00000	0.56351
Cl	0.00000	0.00000	-2.39465

iii) **Cl**Br

Cl	0.00000	0.00000	-0.25967
Br	0.00000	0.00000	1.88107
Cl	0.00000	0.00000	-3.61312

iv) Cl**Br**

Cl	0.00000	0.00000	2.41260
Br	0.00000	0.00000	0.26821
Cl	0.00000	0.00000	-2.96481

v) CF_2**Cl**$_2$

C	-0.06229	-1.35638	0.00000
F	-0.66548	-1.86217	1.07776
Cl	1.62703	-1.83935	0.00000
Cl	-0.23493	0.39045	0.00000
F	-0.66548	-1.86217	-1.07776
Cl	-0.66548	3.89933	0.00000

vi) CF**Cl**$_3$

C	-1.12344	-0.00000	0.26929
F	-1.44836	0.00000	1.57330
Cl	0.63084	-0.00148	0.13023
Cl	-1.80039	1.44728	-0.47190
Cl	-1.80289	-1.44579	-0.47252
Cl	4.13572	0.00000	-0.11377

vii) CF_3**Br**

C	1.73000	-0.00000	-0.00000
Br	-0.18100	0.00000	0.00000
F	2.19400	-0.69200	1.03400
F	2.19400	-0.55000	-1.11700
F	2.19400	1.24200	0.08200
Cl	-3.72200	-0.00000	-0.00000

viii) CF_3**I**

I	-0.21800	-0.00000	0.00000
C	1.91200	0.00000	-0.00000
F	2.38300	0.55900	-1.11300
F	2.38300	0.68500	1.04000
F	2.38300	-1.24300	0.07200
Cl	-3.78000	0.00000	-0.00000

ix) Cl**I**

I	0.00000	0.00000	0.17369
Cl	0.00000	0.00000	2.50382
Cl	0.00000	0.00000	-3.04533

x) **Cl**I

I	0.00000	0.00000	1.57880
Cl	0.00000	0.00000	-0.74363
Cl	0.00000	0.00000	-4.17852